QM-4: Quantum Recipe (from the last class)

Here are the steps we use to solve a problem in Quantum Mechanics:
(assuming a 1D time independent potential energy)

1. Specify the potential energy, $U(x)$.

2. Put $U(x)$ in the TISE:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + U(x)\psi(x) = E\psi(x)$$

3. Solve the TISE for the allowed energies, E, and wavefunctions, $\psi(x)$. These usually form a set E_n and ψ_n. (n is a set of integers)

4. Extract physical information from the wavefunction, $\psi(x)$.

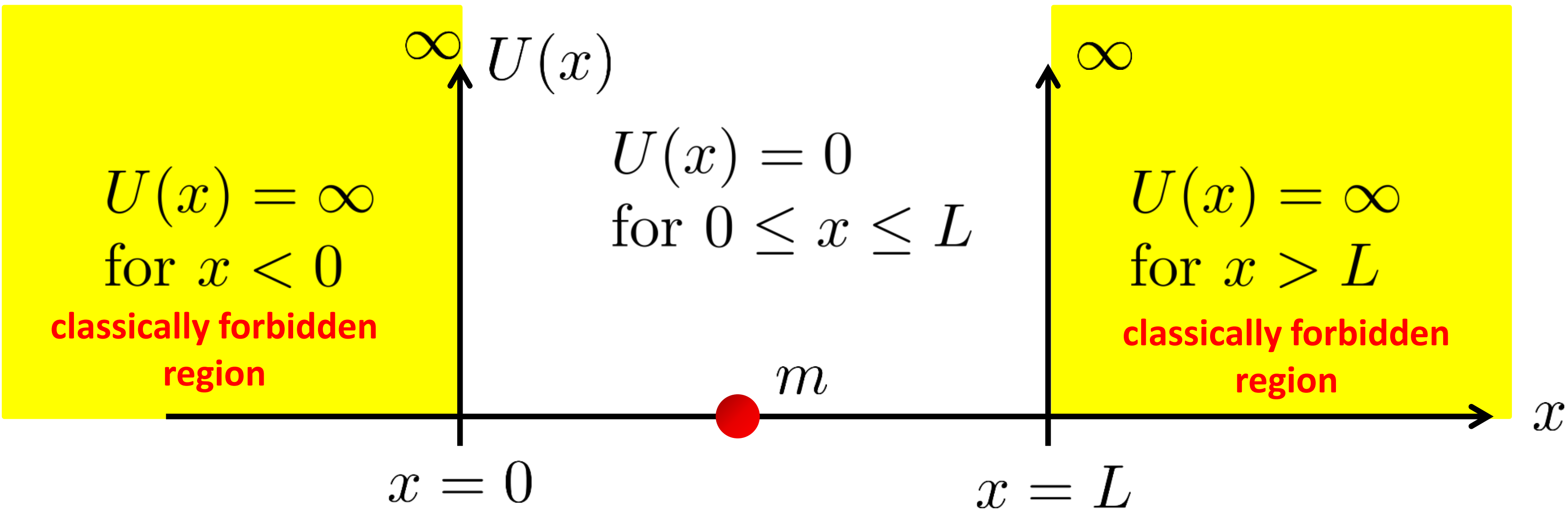
How do we do this last part? →

We looked at how to do some things in Step # 4 in the last class.
Now, let's try Steps 1 - 3 for a real quantum mechanics problem.

The Quantum 1D Infinite Square Well (ISW)

The only "*simple*" problem in quantum mechanics is the **infinite square well**. It is also called "*a particle in a rigid box*", and even though it's relatively easy, there are many important applications of the solution.

The one dimensional ISW is defined by the following Potential Energy:



So, this is **step 1 of the Quantum Recipe** (see previous slide). Before we begin to solve the Schrodinger Equation, **what do de Broglie and HUP tell us to expect?**

de Broglie says that the allowed wavefunctions for the particle will form standing waves inside the well, and HUP says that since the uncertainty in x is the width of the well, the minimum energy of the particle will not be zero. Will Schrodinger agree?

The ISW Solution: Guided Whiteboard QM-12

Step 0: **Draw the 1D well from the previous slide on your whiteboard.**

Step 1: **Find the wavefunction for x < 0 and x > L:**

$$\text{Outside the well } (x < 0 \text{ or } x > L)\text{: } U(x) = \infty$$

Therefore, there is no chance to find the particle there.

$$\text{So, } \psi(x) = 0 \text{ for } x < 0 \text{ or } x > L$$

Step 2: **Write down the Time Independent Schrodinger Equation inside the well.**

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + U(x)\psi(x) = E\psi(x)$$

$$\text{Inside the well } (0 \leq x \leq L)\text{: } U(x) = 0$$

$$\text{So, } -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

The ISW Solution: Guided Whiteboard-12

Step 3: **Simplify the TISE by putting all constants on one side of the equation.**

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \equiv -k^2\psi$$

***What is k?**

***Don't confuse:**
K **= kinetic energy**
k **= wave number**

remember, $U = 0$ and $E = K + U = K$

so, $k^2 = \frac{2mE}{\hbar^2} = \frac{2mK}{\hbar^2} = \frac{2m}{\hbar^2}\frac{p^2}{2m} = \frac{p^2}{\hbar^2}$

Thus k is our old friend the wavenumber, $k = \frac{2\pi}{\lambda}$

Step 4: **Solve the differential equation:** $\frac{d^2\psi}{dx^2} = -k^2\psi$

Wait a minute! Have we seen this equation before?

Yes, it's the same differential equation as for the classical simple harmonic oscillator! The quantities are different (this is a different k), but the equation is the same. ***So, we don't have to solve it again!*** *We can just write down the solution, but let's write it in a slightly different way:*

$$\psi(x) = A\sin kx + B\cos kx$$

Where: A and B are constants that we have to determine.

The ISW Solution: Guided Whiteboard-12

Next, we have to apply the **Boundary Conditions** and the **Normalization Condition** on the wavefunction to find the constants A and B.

The Boundary Conditions are: $\psi(x)$ must be continuous for all x

$$\Rightarrow \psi(x=0)=0 \text{ and } \psi(x=L)=0$$

Step 5: **Apply the boundary condition at x = 0.**

$$\psi(x=0)=0=A\sin(0)+B\cos(0)=B$$

$$\text{So, } B \text{ must } =0, \text{ and } \psi(x)=A\sin kx$$

Step 6: **Apply the boundary condition at x = L** (*No, you don't get A = 0, look for something else and see where this takes you*).

$$\psi(x=L)=0=A\sin kL$$

{ if we set A=0, the wavefunction is zero everywhere, which is not very interesting; there's another possibility }

$$\sin kL=0 \Rightarrow kL=n\pi \Rightarrow k=\frac{n\pi}{L}$$

$$n=1,2,3,\cdots$$

Now, what does this give us?

$$E=\frac{p^2}{2m}=\frac{\hbar^2k^2}{2m}=\frac{\hbar^2n^2\pi^2}{2mL^2}$$

Or, $$E_n=\frac{n^2h^2}{8mL^2}$$

The allowed energy levels! (do these look familiar?)

The ISW Solution: Guided Whiteboard-12

So, we have found the quantized allowed energy levels for the particle, but we still have one undetermined constant in the wavefunction which we can write as:

$$\psi(x) = A\sin kx = A\sin\frac{n\pi x}{L} \qquad \text{since } k = \frac{n\pi}{L}$$

Step 7: **Use the Normalization Condition to find the constant A.** **(LC for 3 points)**

Normalization means: $$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1 = A^2 \int_0^L \sin^2\frac{n\pi x}{L} dx$$

If you're good at doing integrals, do it; or look in an integral table (appendix A):

$$\int \sin^2 ax = \frac{x}{2} - \frac{\sin 2ax}{4a} \qquad a = \text{constant}$$

So, our integral is: $$1 = A^2\left[\frac{x}{2} - \frac{1}{4(\frac{n\pi}{L})}\sin(\frac{2n\pi x}{L})\right]_{x=0}^{x=L}$$

$$= A^2\left[\left(\frac{L}{2} - \frac{L}{4n\pi}\sin(2n\pi)\right) - \left(0 - \frac{L}{4n\pi}\sin(0)\right)\right]$$

$$= A^2\frac{L}{2}$$

$$\text{So, } A = \sqrt{\frac{2}{L}}$$

The ISW Solution: Guided Whiteboard-12

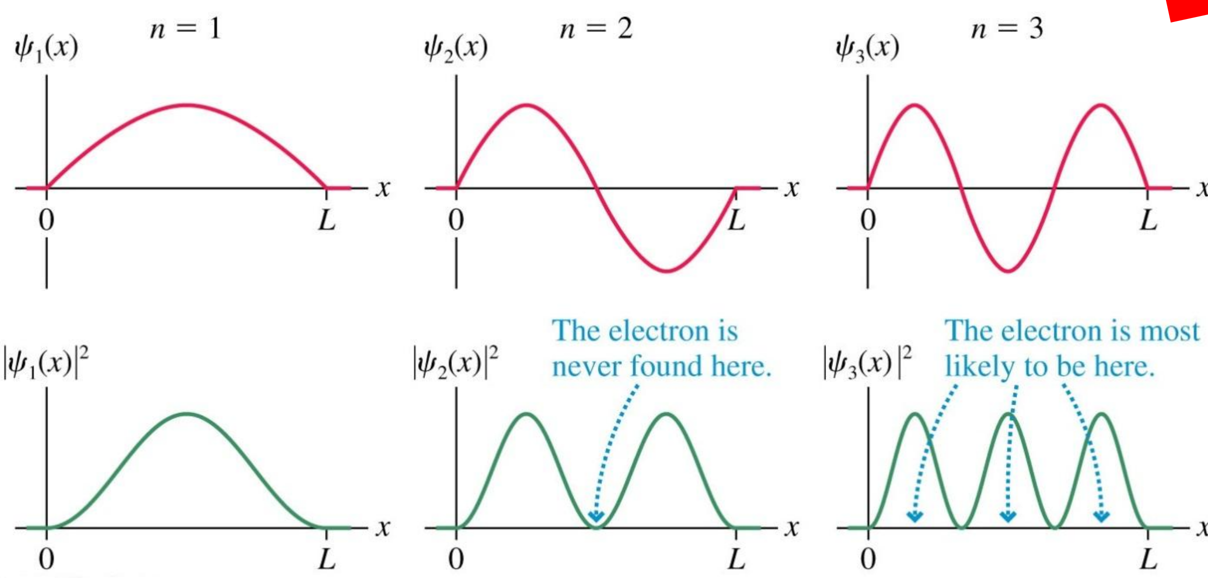
Step 9: Write down the final result: i.e. the wave functions and energies for the ISW.
Shake hands with the other members of your group – you have solved your first quantum mechanics problem! ***Get Your Sticker and proudly display it!***

$$\left.\begin{aligned}\psi_n(x) &= \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} \\ E_n &= \frac{n^2h^2}{8mL^2} = n^2E_1\end{aligned}\right\} n = 1, 2, 3, \cdots$$

What do these wavefunctions look like?

$\psi_n(x)$

$|\psi_n(x)|^2$



Same **wavefunctions** and allowed energy levels that we got fitting standing deBroglie waves into the well.

The Probability Densities, $|\psi_n(x)|^2$

Whiteboard Problem: QM-13

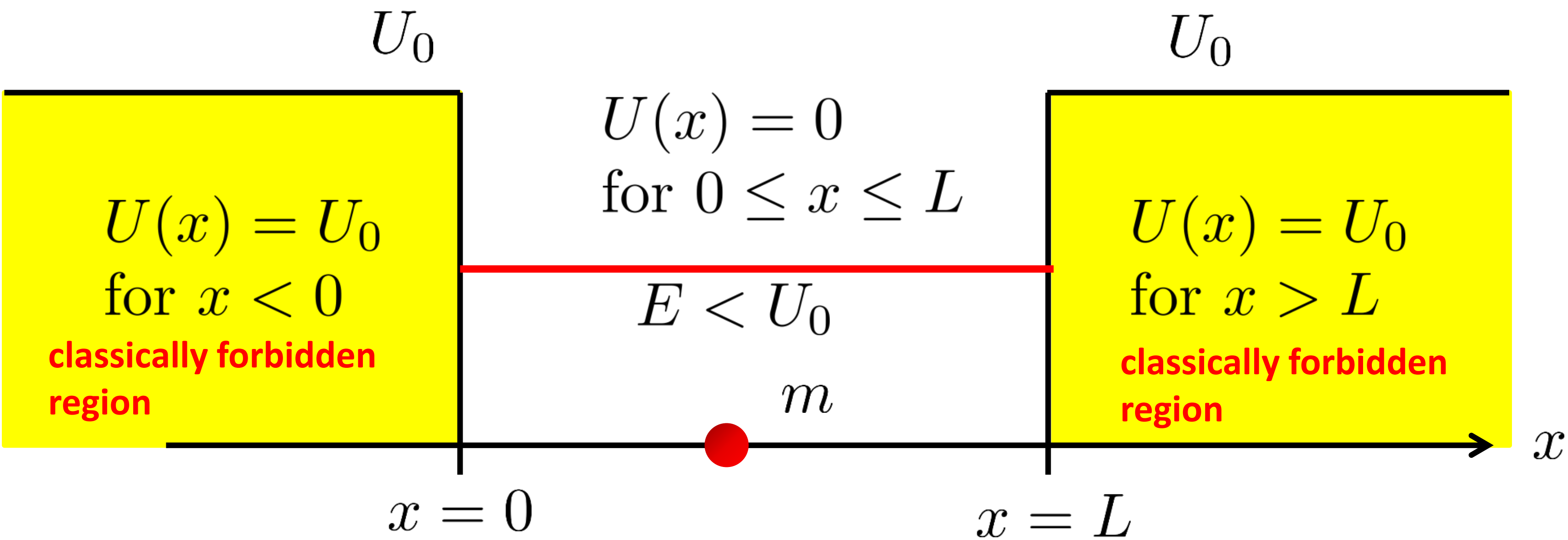
Consider a particle of mass m in a one dimensional infinite square well of width L.

a) **Find an expression for the wavelength of light emitted by the particle when it makes a quantum jump from the n = 2 state to the n=1 state. (LC)**

b) **If this is an electron, what width of the well will give a photon wavelength of 694 nm for the n = 2 to n = 1 transition? (LC)**

The Quantum 1D Finite Square Well

Here, the potential energy well has a finite height, U_0:

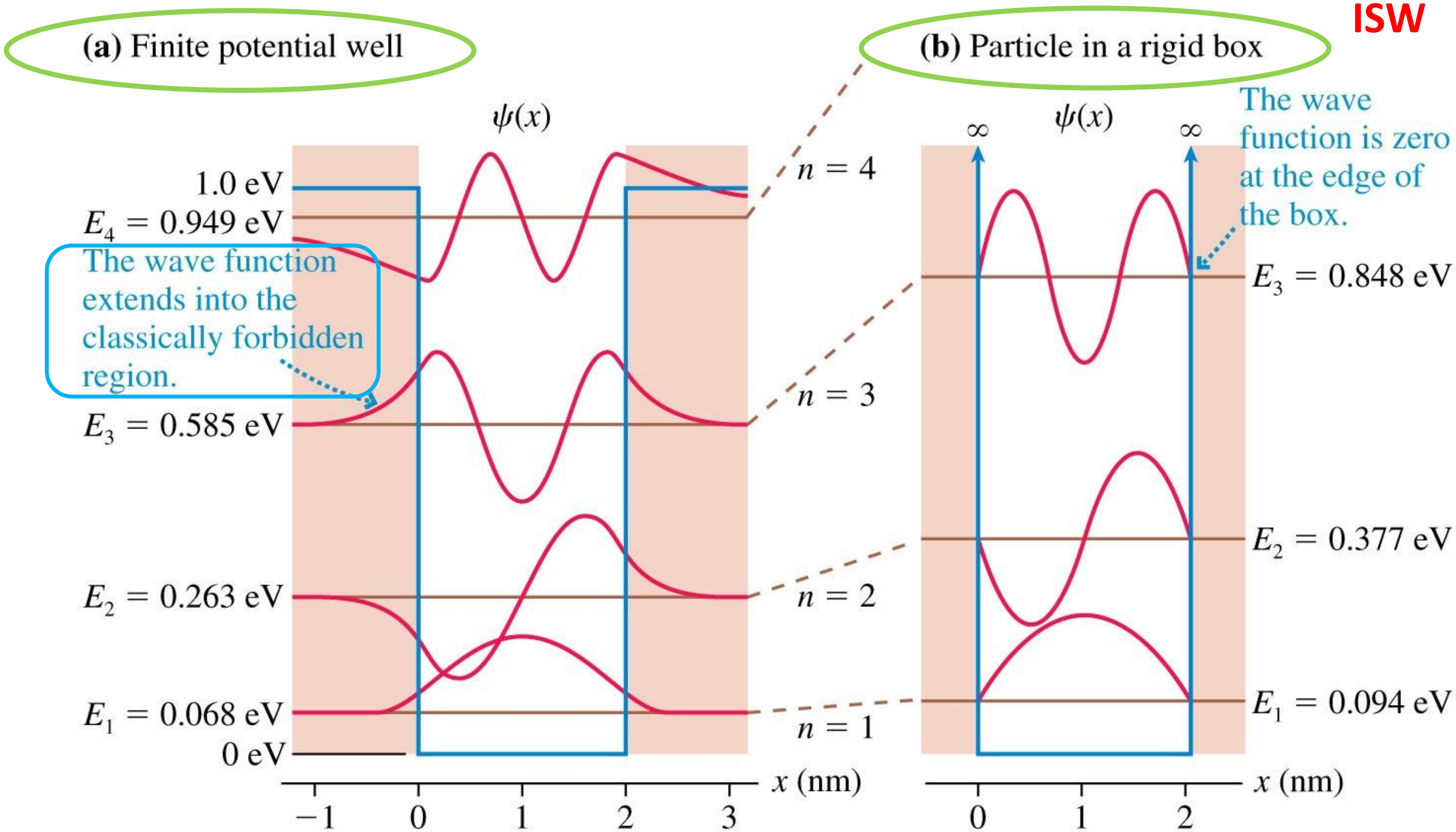


For a particle of mass m in this box with $E < U_0$:

There are still quantized bound states that are similar to the infinite square well, but there are significant differences. This is a fairly tough problem to solve (although, you follow the same quantum recipe), so we'll do as your author does and just look at an example:

The Quantum 1D Finite Square Well: Example

In your text is a graphical solution of an electron trapped in a square well that has width 2.0 nm and a height of 1.0 eV.

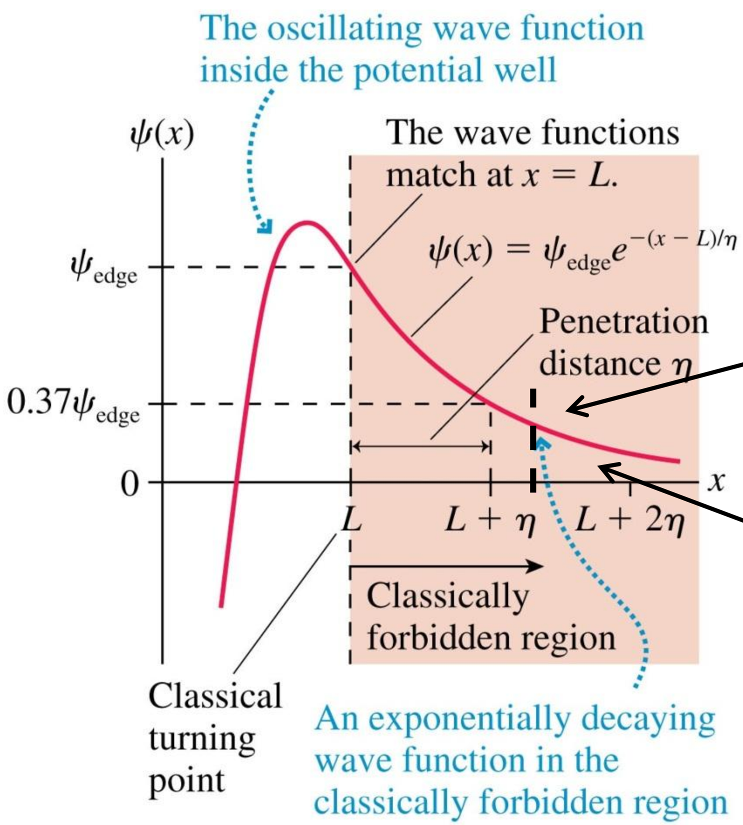


There are a finite number of bound states and the energies are below those for the ISW. The wave functions are similar to the ISW, **but with one big difference: they extend into the classically forbidden region where** $K = E - U_0 < 0$ **Negative kinetic energy!**

The Quantum 1D Finite Square Well: Penetration Depth

How far does the wavefunction penetrate into the classically forbidden region?

The wavefunction decays exponentially, but your author derives an approximate expression for the **penetration depth - the distance for the wave function to decay by a factor of 1/e:**



The penetration depth is:

$$\eta = \frac{\hbar}{\sqrt{2m(U_0 - E)}}$$

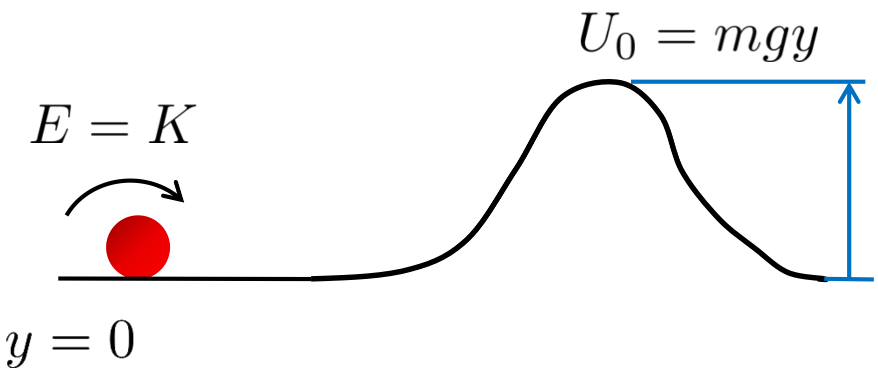
What would happen if the potential energy came back to zero before the wavefunction decayed to zero?

The wavefunction would then return to being an oscillating function here with reduced amplitude, and we would have the possibility of finding the particle there with non-zero probability. This is called:
<u>"Quantum Tunneling."</u>

Potential Barriers

A potential barrier is a region of increased potential energy that an object can go over, reflect from, or in quantum mechanics, magically tunnel through!

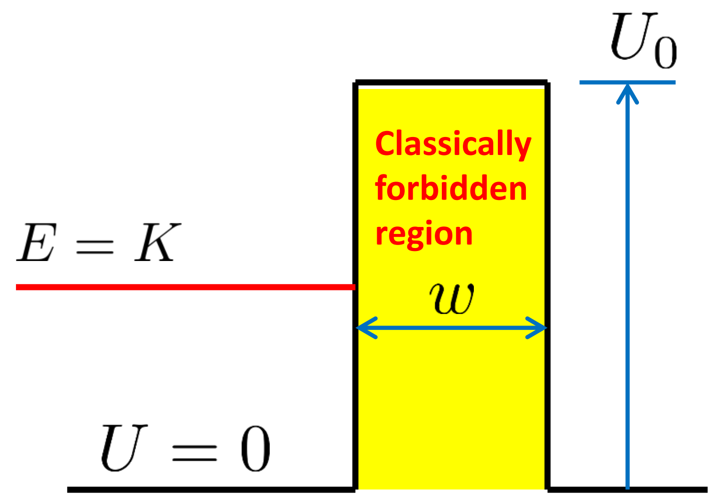
A Barrier in a Gravitational PE:



For $K < U_0$ Ball rolls partway up the hill, then comes back where it came from, i.e. reflected.

For $K > U_0$ Ball rolls over the hill and comes out on the other side with same KE.

An Idealized Potential Barrier:



From what we learned in Chapters 9 and 10, unless

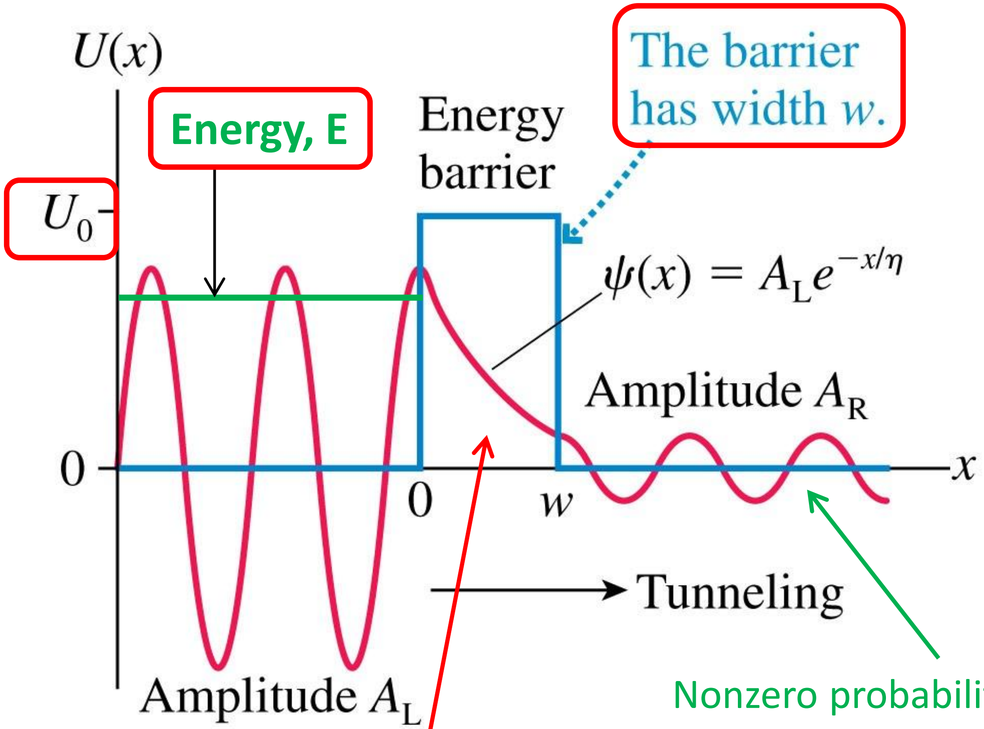
$$E > U_0$$

the object will always reflect from the barrier. **But in the Quantum World . . . .**

[a great video by Maryam Tsegaye](#).

Quantum Tunneling

Tunneling is a uniquely quantum phenomenon. ***As Maryam said, "it's as if you walked into a brick wall, and instead of bouncing backwards, you magically appeared on the other side of the wall!"*** Things like this don't happen in the classical world, but they are very common in the quantum world. Consider the wavefunction below:



Nonzero probability that the particle is here

Wavefunction decays exponentially inside the barrier, but the barrier ends before it decays to zero.

The probability that the particle with mass m and energy E will tunnel through the barrier of width w is approximately:

$$P_{\text{tunnel}} = e^{-\frac{2w}{\eta}}$$

Where the penetration depth is:

$$\eta = \frac{\hbar}{\sqrt{2m(U_0 - E)}}$$

PhET tunneling

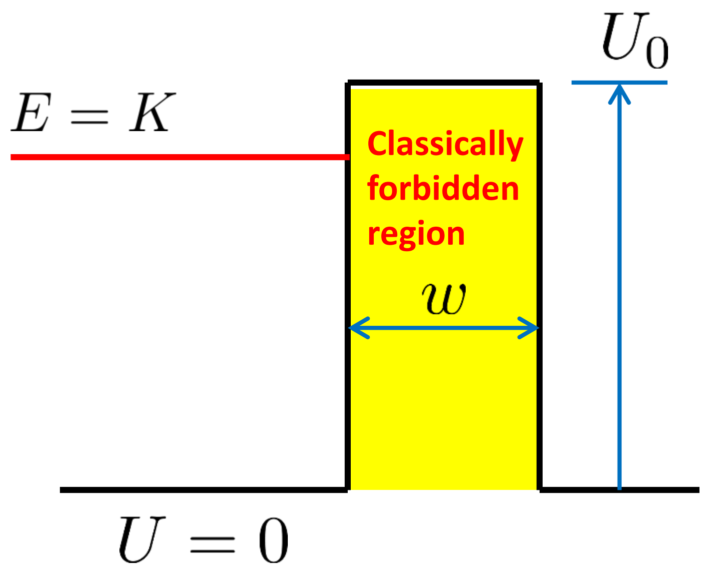
(how do you interpret these wave packets?)

Whiteboard Problem QM-14

(tunneling in the quantum world is easy!)

An electron with energy E = K = 4.8 eV approaches a w = 1.0 nm wide potential energy barrier of height U_0 = 5.0 eV.

Calculate the probability that the electron will tunnel through the barrier. **(LC)**



$$P_{\text{tunnel}} = e^{-\frac{2w}{\eta}}$$

$$\eta = \frac{\hbar}{\sqrt{2m(U_0 - E)}}$$

The most ridiculous **Whiteboard Problem: QM-15**

(tunneling in the classical world is not easy!)

What is the probability that a tennis ball will tunnel through the strings of a tennis racket?

Tennis players routinely hit tennis balls travelling more than 100 mph; however, at some sufficiently high speed, the ball will break through the strings. **Model the racket as a rectangular potential energy barrier whose height is the energy of the slowest moving ball that will just break the strings. Suppose that a 100 g tennis ball traveling at v_{max} = 200 mph is just sufficient to break the 2 mm thick strings.**

Estimate the probability that a 120 mph ball will tunnel through the racket without breaking the strings. Give your answer as a power of 10 rather than a power of *e*. (LC, a 3-point shot)

Hint: estimate the potential energy barrier as $U_0 = \frac{1}{2}mv_{\max}^2$

Answer: $10^{-1.18\times10^{32}}$

This has to be the most ridiculously small number that you've ever seen, but it's not zero!

And yet, tunneling in the quantum world happens all the time. It is necessary to explain certain types of radioactive decay and it is also necessary to explain the Hydrogen fusion reactions that power the Sun.

Do You Want More Quantum Mechanics?

(Perhaps you've heard of Quantum Information or Quantum Computing.)

PHY 281. Contemporary Physics I: Foundations. (3) **Offered only in Fall Semesters**

The course emphasizes special relativity and quantum physics, and the development of quantitative problem-solving skills necessary for the application of advanced physics concepts. The PHY 281/282 sequence provides a solid conceptual and mathematical foundation for students continuing with advanced physics courses. It is also valuable as a terminal physics sequence for students in physics-related fields.

Prerequisite: PHY 182.

Co-requisite: MTH 252 (or permission of instructor).